On the effect of interactions beyond nearest neighbours on non-convex lattice systems

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ON THE EFFECT OF INTERACTIONS BEYOND NEAREST NEIGHBOURS ON NON-CONVEX LATTICE SYSTEMS

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Abstract. We analyse the rigidity of non-convex discrete energies where at least nearest and next-to-nearest neighbour interactions are taken into account. Our purpose is to show that interactions beyond nearest neighbours have the role of penalising changes of orientation and, to some extent, they may replace the positive-determinant constraint that is usually required when only nearest neighbours are accounted for. In a discrete to continuum setting, we prove a compactness result for a family of surface-scaled energies and we give bounds on its possible Gamma-limit in terms of interfacial energies that penalise changes of orientation.

Keywords: Nonlinear elasticity, Discrete to continuum, Geometric rigidity, Next-to-nearest neighbours, Gamma-convergence.
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Introduction

In the simplest model of atomistic interactions, the behaviour of a system of n particles is described by pair interaction energies of the form

$$\sum_{1\le i\neq j\le n} J(|u_i-u_j|)\,,$$

where i and j label the pair of atoms, and u_i and u_j denote the corresponding positions. Typically, the interatomic potential J is assumed to be repulsive at small distances and attractive at long distances, such as the celebrated Lennard-Jones potential. Numerical results (see for example [27] and references therein) suggest that equilibrium configurations for such systems arrange approximately in a periodic lattice as the number of particles increases (crystallisation). The problem of crystallization for interactions of Lennard-Jones type is still open. A contribution in this direction has been given in [26], where it is proved, in two dimensions, the optimality under compact perturbations of the equilateral triangular lattice.

Assuming that we have crystallization on some reference lattice $\mathcal{L}$, it is reasonable to suppose that for some class of problems the positions $u_1,\dots,u_n$ are close to $\mathcal{L}$, and then consider lattice energies parametrised on $\mathcal{L}$. A further simplification is to assume that the energy densities themselves depend on the labels i,j; in this context a discrete-to-continuum limit can be performed by interpreting functions defined on $\mathcal{L}$ as traces of functions defined in the continuum, and a macroscopic energy can be derived. The coarser simplification is when only nearest neighbours are taken into account (i.e., we set the interaction energy to zero if i,j are not nearest neighbours in $\mathcal{L}$).

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However, such an oversimplification is usually in contrast with the assumption that ground states are still close to $\mathcal{L}$, since it may yield new undesirable ground states obtained, e.g., by locally changing the orientation of the reference lattice. In order to overcome this, either the energy J must be modified, or some other assumptions added. A possible choice is to consider longer range interactions (e.g., second neighbours, etc.). Another choice is to add a restriction on the deformation u corresponding to the local non-interpenetration condition $\det \nabla u > 0$. However, imposing a positive-determinant constraint on lattice systems gives rise to analytical difficulties in deriving the continuum limit by a variational approach. Moreover, this condition may not be preserved in the limit. For an extended discussion on these issues we refer to [8], where the authors show some pathological effects that call into question the necessity of such an assumption.

The purpose of this paper is to analyse discrete systems when next-to-nearest neighbour interactions, and, more in general, interactions in a finite range are taken into account. We show that, to some extent, their effect may replace the positive-determinant constraint in penalising changes of orientation, which are thus not excluded by assumption but rather energetically disfavoured.

We point out that the effects of long range interactions in non-convex lattice systems have already been treated in some papers in the one-dimensional case. A first variational analysis has been proposed in [13], which considers nearest and next-to-nearest interactions of quadratic type, showing the appearance of external boundary layers. A complete study in dimension one through a discrete-to-continuum analysis has been subsequently carried out in [6], which studies a development by Γ-convergence for non-convex interactions, characterising external and internal boundary layers and in particular rigorously showing the equivalence with higher-order Modica-Mortola type perturbed energies; see also [22, 23]. It is worth mentioning the paper [10], where next-to-nearest neighbour interactions replace the monotonicity assumption made in [9] for deriving Griffith energies from Lennard-Jones interactions. In the higher-dimensional case, a first contribution was given in [4], where the authors deduce a formal (pointwise) development of the energies in terms of the lattice spacing as a singular perturbation of an elastic energy with a term containing second derivatives.

In our paper we study the problem in the higher-dimensional case by means of a variational convergence. We will restrict our attention to interaction potentials that satisfy polynomial growth conditions (i.e., strongly attractive at long distances), mimicking the behaviour of Lennard-Jones type potentials at short distances and leading in the macroscopic limit to continuum elastic theories that do not allow for fractures. We believe that, even under this restriction, our analysis highlights interesting phenomena and provides an essential step towards the understanding of more general Lennard-Jones type potentials.

Assuming the existence of a reference configuration identified with a portion $\mathcal{L}'$ of a periodic lattice $\mathcal{L}$ in $\mathbb{R}^N$, the deformation map can be regarded as a function $u\colon \mathcal{L}' \to \mathbb{R}^N$. As a model case, we consider energies of the form

$$\sum_{|i-j|\le R} \left(|u_i - u_j| - |i-j|\right)^2, \tag{0.1}$$

where R is a positive constant larger than the lattice spacing. The constant R determines the range of interactions contributing to the energy functional and is to be chosen according to the lattice under examination. A prototypical example is the two-dimensional case of particles sitting on a triangular lattice in their reference configuration and interacting via harmonic springs between nearest and next-to-nearest neighbours. More precisely, normalising the equilibrium

distance of the particles to one, the reference configuration $\mathcal{L}'$ is a portion of the triangular Bravais lattice $\mathbb{Z}v_1 \oplus \mathbb{Z}v_2$, where $v_1 = (1, 0)$ and $v_2 = (1/2, \sqrt{3}/2)$, and the corresponding total internal energy is of the form (0.1) with $R = \sqrt{3}$.

Note that, up to translations, the ground states of energies of the type (0.1) are given by all linear maps in $O(N)$, while adding a positive-determinant constraint reduces them to $SO(N)$. Nonetheless, the presence of next-to-nearest neighbour or longer range interactions prevents the appearance of many changes of orientation, since these are energetically disfavoured. In contrast, it can be easily shown that the sole presence of nearest neighbour interactions allows changes of orientation without any additional cost.

By scaling the reference lattice $\mathcal{L}$ by a small parameter $\varepsilon > 0$ and identifying $\mathcal{L}'$ with $\varepsilon\mathcal{L} \cap \Omega$, where Ω is a bounded open set in $\mathbb{R}^N$, one can consider a bulk scaling of (0.1) and rewrite it in terms of difference quotients, thus obtaining functionals of the form

$$F_\varepsilon(u) := \sum_{|i-j|\le R} \varepsilon^N \left(\frac{|u_i - u_j|}{\varepsilon} - |i-j| \right)^2 , \tag{0.2}$$

where we use the notation $u_i := u(\varepsilon i)$. The asymptotic behaviour of F_ε, as ε tends to zero, was studied in [1] by means of Γ-convergence (see [5, 16]) and leads to a continuum limit described by a functional of the form $\int_\Omega f(\nabla u)\,\mathrm{d}x$ defined on some Sobolev space. Here f is a non-negative quasi-convex function, that is zero on $O(N)$; therefore, the set of minimisers of f contains the quasi-convex hull of $O(N)$ and thus, in particular, all rank-one segments between $SO(N)$ and $O(N) \setminus SO(N)$. Indeed, in the bulk scaling regime, rotations and reflections can be mixed with a negligible cost in the limit.

Even though this result gives some insight into the structure of the equilibria of F_ε, encoded in the formula defining the density f, the effect of long range interactions in penalising changes of orientation takes place at a surface scale which is not detected by this analysis. Hence a higher order description is needed, which can be achieved by studying the asymptotic behaviour of the surface-scaled energies

$$E_\varepsilon(u) := \varepsilon^{-1} F_\varepsilon(u)\,. \tag{0.3}$$

We prove a compactness result (Theorem 3.1), asserting that the gradient of the limit of a sequence u_ε for which $E_\varepsilon(u_\varepsilon)$ is uniformly bounded, is piecewise constant with values in $O(N)$ and that the underlying partition of Ω consists of sets of finite perimeter. Key mathematical tools in its proof are the well-known rigidity estimate of Friesecke, James, and Müller [17] and the piecewise rigidity result proven by Chambolle, Giacomini, and Ponsiglione in [12].

The compactness result provided by Theorem 3.1 has applications also in problems of dimension reduction, for example it is used in [2] to prove scaling properties of energies in nanowires, in particular it allows to extend the results of [19, 20] by removing the positive-determinant constraint.

The characterisation of the Γ-limit of (0.3) turns out to be a rather delicate problem. Propositions 4.1 and 4.4 provide bounds on the Γ-limit in terms of interfacial energies that penalise changes of orientation. More precisely, denoting by E the Γ-limit of a subsequence of $\{E_\varepsilon\}$, we show that, for each $u \in W^{1,\infty}(\Omega;\mathbb{R}^N)$ such that $\nabla u \in SBV(\Omega; O(N))$,

$$E(u) \ge \int_{J_{\nabla u}} g_1(\nu_{\nabla u})\,\mathrm{d}\mathcal{H}^{N-1}\,. \tag{0.4}$$

Here $J_{\nabla u}$ denotes the jump set of ∇u, $\nu_{\nabla u}$ is the unit normal to $J_{\nabla u}$, while g_1 is defined by a suitable asymptotic formula and is bounded from below by a positive constant (see Remark

4.2). An analogous upper bound holds for the class $\mathcal{W}(\Omega)$ of limiting deformations u such that $J_{\nabla u}$ is a polyhedral set, that is, it consists of the intersection of Ω with the union of a finite number of $(N-1)$-dimensional simplices of $\mathbb{R}^N$. Namely, we have

$$E(u) \leq \int_{J_{\nabla u}} g_2(\nu_{\nabla u})\, \mathrm{d}\mathcal{H}^{N-1} \quad \text{for all } u \in \mathcal{W}(\Omega)\,, \tag{0.5}$$

where g_2 is the limit of a sequence of suitable Dirichlet minimum problems and it is uniformly bounded from above by a positive constant. Thus, the continuum limit penalises the jump set $J_{\nabla u}$ and, at least on the class $\mathcal{W}(\Omega)$, is concentrated on $J_{\nabla u}$. By rotational invariance, the density of a possible integral representation of the Γ-limit of E_ε would depend only on $\nu_{\nabla u}$. However, its computation remains an open question and leads to interesting analytical issues. Indeed, a standard argument to show that (0.4) and (0.5) are optimal bounds and that $g_1 = g_2$ amounts to prove that it is possible to modify the boundary values of optimising sequences with a negligible energy cost. This does not seem a trivial task in the present context. Another interesting question, in analogy with density results in BV spaces, is whether any admissible limiting deformation u can be approximated by a sequence of regular deformations $u_n \in \mathcal{W}(\Omega)$, so that $\int_{J_{\nabla u_n}} g_2(\nu_{\nabla u_n})\, \mathrm{d}\mathcal{H}^{N-1}$ converges to the corresponding energy of u. Indeed, by the lower semicontinuity of the Γ-limit, this would allow us first to extend the upper estimate (0.5) to the whole limiting domain, and second, in combination with a positive answer to the first question, to provide a complete characterisation of the Γ-limit.

We point out that including long range interactions in lattice energies has a similar effect to that of adding higher-order perturbations in continuum models (cf. the above mentioned papers [4, 13, 6]). The presence of higher-order perturbations brings in considerable technical difficulties also in the continuum case. In fact, our discrete model is closely related to the classical double-well singularly perturbed functionals studied in the context of gradient theories for phase transitions (see e.g. [14, 15]), where one considers energies of the form

$$\int_\Omega \frac{1}{\varepsilon} W(\nabla u) + \varepsilon |\nabla^2 u|^2 \, \mathrm{d}x\,. \tag{0.6}$$

Here W is a non-negative function vanishing on the set $K := SO(N)A \cup SO(N)B$, where A and B are given rank-one connected matrices with positive determinant. The second order term in (0.6) has the role of penalising oscillations between the two wells as in our discrete model long range interactions penalise oscillations between $SO(N)$ and $O(N)\backslash SO(N)$. In [15] it is shown that the Γ-limit of (0.6) is an interfacial energy concentrated on the jump set of ∇u. A microscopic derivation of such result has been recently obtained in [18] in the context of square-to-rectangular martensitic phase transitions. We point out that in [15, 18] the two wells of K consist of matrices with positive determinant, while this is not the case in the present context. Such difference is at the origin of the difficulties highlighted above.

Notation. We recall some basic notions of geometric measure theory for which we refer to [3]. Given a bounded open set $\Omega \subset \mathbb{R}^N$, $N \geq 2$, and $M \geq 1$, $BV(\Omega;\mathbb{R}^M)$ denotes the space of functions of bounded variation; i.e., of functions $u \in L^1(\Omega;\mathbb{R}^M)$ whose distributional gradient $\mathrm{D}u$ is a Radon measure on Ω with $|\mathrm{D}u|(\Omega) < +\infty$, where $|\mathrm{D}u|$ is the total variation of $\mathrm{D}u$. If $u \in BV(\Omega;\mathbb{R}^M)$, the symbol ∇u stands for the density of the absolutely continuous part of $\mathrm{D}u$ with respect to the N-dimensional Lebesgue measure $\mathcal{L}^N$. We denote by J_u the jump set of u, by u^+ and u^- the traces of u on J_u, and by $\nu_u(x)$ the measure theoretic normal to J_u at x, which is defined for $\mathcal{H}^{N-1}$-a.e. $x \in J_u$, where $\mathcal{H}^{N-1}$ is the $(N-1)$-dimensional Hausdorff measure. A function $u \in BV(\Omega;\mathbb{R}^M)$ is said to be a special function of bounded variation if $\mathrm{D}u - \nabla u\, \mathcal{L}^N$ is

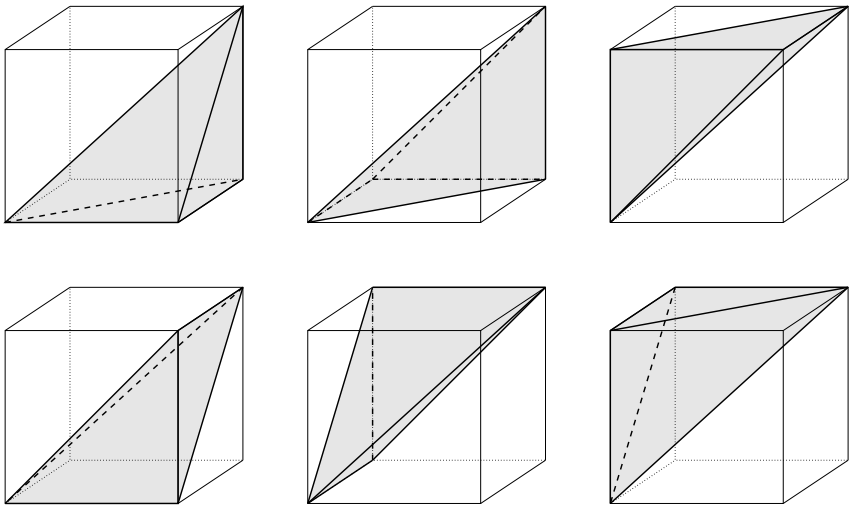


Figure 1: The six tetrahedral elements of the Kuhn decomposition of a cube in dimension three.

concentrated on J_u; in this case one writes $u \in SBV(\Omega;\mathbb{R}^M)$. Given a set $E \subset \Omega$, we denote by $P(E,\Omega)$ its relative perimeter in Ω and by $\partial^* E$ its reduced boundary.

For $N \geq 2$, $\mathbb{M}^{N\times N}$ is the set of real $N\times N$ matrices, $GL^+(N)$ is the set of matrices with positive determinant, $O(N)$ is the set of orthogonal matrices, and $SO(N)$ is the set of rotations. We denote by I the identity matrix and J the reflection matrix such that $Je_1 = -e_1$ and $Je_i = e_i$ for $i = 2,\dots,N$, where $\{e_i\colon i = 2,\dots,N\}$ is the canonical basis in $\mathbb{R}^N$. Moreover, given $N+1$ points $x_0, x_1, \dots, x_N \in \mathbb{R}^N$, we denote by $[x_0, x_1, \dots, x_N]$ the simplex determined by all convex combinations of those points.

In the paper, the same letter C denotes various positive constants whose precise value may change from place to place.

1. Setting of the problem

We study the deformations of a Bravais lattice governed by pairwise potentials with finite range interactions. Up to an affine deformation $H \in GL^+(N)$, we can reduce to the case where the lattice is $\mathbb{Z}^N$. (See Remark 2.6 for details on the treatment of some specific lattices in dimension two and three.) In order to define the interaction energy, we introduce the so-called Kuhn decomposition, denoted by $\mathcal{T}$, which consists in a partition of $\mathbb{R}^N$ into N-simplices. First we define a partition $\mathcal{T}_0$ of the unit cube $(0,1)^N$ into N-simplices: we say that $T \in \mathcal{T}_0$ if the $(N+1)$-tuple of its vertices belongs to the set

$$\left\{ \{0, e_{i_1}, e_{i_1}+e_{i_2}, \dots, e_{i_1}+e_{i_2}+\cdots+e_{i_N}\}\colon \begin{pmatrix} 1 & 2 & \cdots & N \\ i_1 & i_2 & \cdots & i_N \end{pmatrix} \in S_N \right\},$$

where S_N is the set of permutations of N elements; see Figure 1. Next, we define $\mathcal{T}$ as the periodic extension of $\mathcal{T}_0$ to all of $\mathbb{R}^N$. We say that two nodes $x, y \in \mathbb{Z}^N$ are contiguous if there exists a simplex $T \in \mathcal{T}$ that has both x and y as its vertices. We set

$$B_1 := \{\xi \in \mathbb{R}^N\colon x \text{ and } x+\xi \text{ are contiguous}\}. \tag{1.1}$$

If both $[x_0, x_1, \dots, x_N]$ and $[y_0, x_1, \dots, x_N]$ belong to $\mathcal{T}$, then we say that $[x_0, x_1, \dots, x_N]$ and $[y_0, x_1, \dots, x_N]$ are neighbouring simplices (i.e., they share a facet) and x_0 and y_0 are opposite vertices. We set

$$B_2 := \{\xi \in \mathbb{R}^N : x \text{ and } x+\xi \text{ are opposite vertices}\}, \tag{1.2}$$

and remark that, by periodicity, B_1 and B_2 do not depend on x.

Let Ω be an open bounded Lipschitz subset of $\mathbb{R}^N$. Given $\varepsilon > 0$ we consider

$$\mathcal{L}_\varepsilon := \varepsilon\mathbb{Z}^N \cap \overline{\Omega}_\varepsilon,$$

where $\overline{\Omega}_\varepsilon$ is the union of all hypercubes with vertices in $\varepsilon\mathbb{Z}^N$ that have non-empty intersection with Ω. We identify every deformation u of the lattice $\mathcal{L}_\varepsilon$ by its piecewise affine interpolation with respect to the triangulation $\varepsilon\mathcal{T}$. By a slight abuse of notation, such extension is still denoted by u. We define the domain of the functional as

$$\mathcal{A}_\varepsilon := \big\{u \in C^0(\overline{\Omega}_\varepsilon;\mathbb{R}^N) : u \text{ piecewise affine}, \\ \nabla u \text{ constant on } \overline{\Omega}_\varepsilon \cap \varepsilon T \ \forall T \in \mathcal{T}\big\}.$$

We remark that all the results are independent of the choice of the interpolation. Indeed, all that follows still holds if one identifies the deformations with their piecewise constant interpolation instead of their piecewise affine interpolation, provided one uses a suitable notion of convergence; see for example [25].

For fixed $p > 1$ and $H \in GL^+(N)$, we study the following surface-scaled discrete energy,

$$E_\varepsilon(u) := \varepsilon^{N-1} \sum_{\xi \in B_1 \cup B_2} \sum_{\substack{x \in \mathcal{L}_\varepsilon \\ x+\varepsilon\xi \in \mathcal{L}_\varepsilon}} \left| \frac{|u(x+\varepsilon\xi)-u(x)|}{\varepsilon} - |H\xi| \right|^p, \tag{1.3}$$

for $\varepsilon > 0$.

Remark 1.1. *Our results generalise to energies of the form*

$$\varepsilon^{N-1} \sum_{\substack{\xi \in \mathbb{Z}^N \\ |\xi| \le R}} \sum_{\substack{x \in \mathcal{L}_\varepsilon \\ x+\varepsilon\xi \in \mathcal{L}_\varepsilon}} \phi\Big(\xi, \frac{|u(x+\varepsilon\xi)-u(x)|}{\varepsilon} - |H\xi|\Big), \tag{1.4}$$

where R is chosen in such a way that $R \ge \max\{|\xi| : \xi \in B_1 \cup B_2\}$, $\phi\colon \mathbb{Z}^N \times \mathbb{R} \to [0, +\infty)$ is a positive potential satisfying polynomial growth conditions in the second variable and such that $\min \phi(\xi, z) = \phi(\xi, 0) = 0$ and $\phi(\xi, z) > 0$ if $z > 0$. For simplicity, here we develop our analysis in detail only in the case of p-harmonic potentials as in (1.3).

2. Discrete rigidity

The following result will play a crucial role in deriving rigidity estimates in our discrete setting. (See [11, 24, 26] for discrete rigidity estimates.)

Theorem 2.1. [17, Theorem 3.1] *Let $N \ge 2$, and let $1 < p < \infty$. Suppose that $U \subset \mathbb{R}^N$ is a bounded Lipschitz domain. Then there exists a constant $C = C(U)$ such that for each $u \in W^{1,p}(U;\mathbb{R}^N)$ there exists a constant matrix $R \in SO(N)$ such that*

$$\|\nabla u - R\|_{L^p(U;\mathbb{M}^{N\times N})} \le C(U) \|\mathrm{dist}(\nabla u, SO(N))\|_{L^p(U)}. \tag{2.1}$$

The constant $C(U)$ is invariant under dilation and translation of the domain.

It is convenient to define the energy of a single simplex T with vertices $x_0, \dots, x_N$,

$$E_{\mathrm{cell}}(u_F; T) := \sum_{i \le j = 0}^{N} \Big| |F(x_i - x_j)| - |H(x_i - x_j)| \Big|^p \quad \text{for every } F \in \mathbb{M}^{N \times N},$$

where u_F is the affine map $u_F(x) := Fx$. The following lemma provides a lower bound on $E_{\mathrm{cell}}(u_F; T)$ in terms of the distance of F from $O(N)$. It will be instrumental in using Theorem 2.1.

Lemma 2.2. *There exists a constant $C > 0$ such that*

$$\mathrm{dist}^p(F, SO(N)H) \le C\, E_{\mathrm{cell}}(u_F; T) \quad \textit{for every } F \in \mathbb{M}^{N \times N} \textit{ with } \det F \ge 0, \tag{2.2a}$$

$$\mathrm{dist}^p(F, (O(N) \backslash SO(N))H) \le C\, E_{\mathrm{cell}}(u_F; T) \quad \textit{for every } F \in \mathbb{M}^{N \times N} \textit{ with } \det F \le 0. \tag{2.2b}$$

Proof. Set $\delta_{ij} := |F(x_i - x_j)| - |H(x_i - x_j)|$ for $i \le j = 0, \dots, N$, so that $E_{\mathrm{cell}}(u_F; T) = \sum_{i \le j = 0}^{N} \delta_{ij}^p$. Assume first that $\mathrm{dist}(F, O(N)H)$ is small and that $\det F \ge 0$. In particular, we can assume $\mathrm{dist}(F, SO(N)H) \le \tau$ where τ is a small parameter whose value will be fixed later. By the equivalence of norms in $\mathbb{R}^{(N+1)(N+2)/2}$, it suffices to prove

$$\frac{1}{C} \mathrm{dist}^2(F, SO(N)H) \le \sum_{i \le j = 0}^{N} \delta_{ij}^2 =: E_2(F).$$

Define RH as the orthogonal projection of F on $SO(N)H$, so that $\mathrm{dist}(F, SO(N)H) = |F - RH|$. By computing the second order Taylor expansion of E_2 about RH and recalling that matrices in $SO(N)H$ are minimum points for E_2, we see that

$$E_2(F) = \frac{1}{2} \nabla^2 E_2(RH)(F - RH, F - RH) + o(|F - RH|^2) \ge C |F - RH|^2 + o(|F - RH|^2),$$

since on $SO(N)H$ the Hessian of E_2 is positive definite on the orthogonal complement of the tangent space of $SO(N)H$ at RH, see e.g. [11, Remark 4]. In the case when $\det F \le 0$ the above argument is repeated replacing $SO(N)$ by $O(N) \backslash SO(N)$. Therefore, if $\mathrm{dist}(F, O(N)H)$ is sufficiently small, then (2.2a) and (2.2b) are readily seen to hold.

On the other hand, if $\mathrm{dist}(F, O(N)H)$ is sufficiently large, (and therefore $\max_{i \le j} |\delta_{ij}|$ is larger than a fixed constant,) then

$$\mathrm{dist}^2(F, SO(N)H) \le |F - H|^2 \le C \sum_{j=1}^{N} |(F - H)(x_j - x_0)|^2,$$

$$\mathrm{dist}^2(F, (O(N) \backslash SO(N))H) \le |F - JH|^2 \le C \sum_{j=1}^{N} |(F - JH)(x_j - x_0)|^2.$$

By the triangle inequality, $|(F - H)(x_j - x_0)| \le |F(x_j - x_0)| + |H(x_j - x_0)| = 2|H(x_j - x_0)| + |\delta_{0j}| \le C \max_{i \le j} |\delta_{ij}|$, and the same holds for $F - JH$; thus (2.2a) and (2.2b) follow. The intermediate cases follow by a continuity argument. □

The next lemma asserts that if in two neighbouring simplices the sign of $\det \nabla u$ has different sign, then the energy of those two simplices is larger than a positive constant. It will be convenient to define the energetic contribution of the interactions within two neighbouring simplices

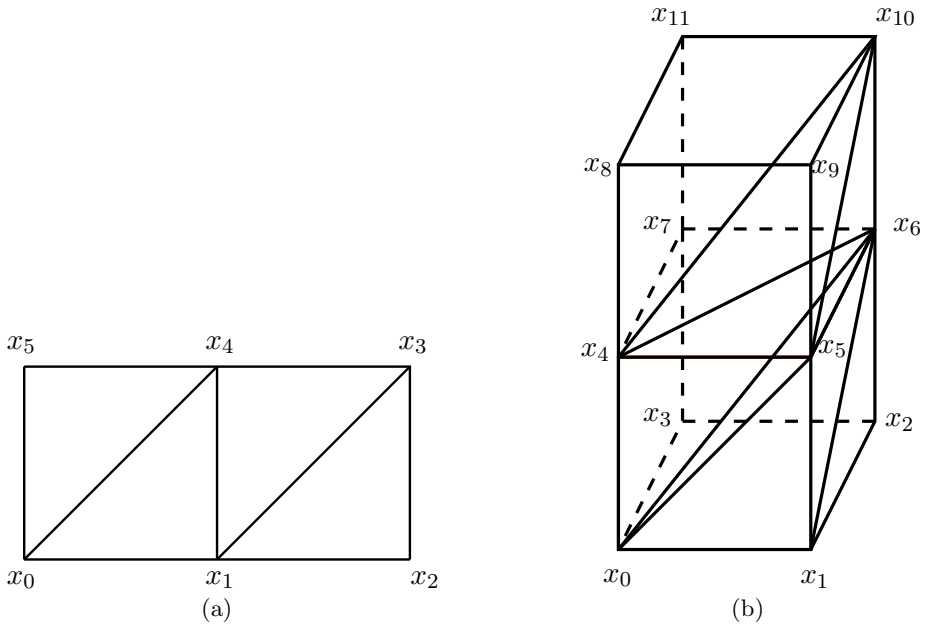


Figure 2: Notation for Remark 2.4.

$T = [x_0, x_1, \dots, x_N]$, $S = [y_0, x_1, \dots, x_N]$ as

$$E_{\text{cell}}(u; S \cup T) := \sum_{i \le j = 0}^{N} \Big| |u(x_i) - u(x_j)| - |H(x_i - x_j)| \Big|^p + \sum_{j=1}^{N} \Big| |u(y_0) - u(x_j)| - |H(y_0 - x_j)| \Big|^p + \Big| |u(y_0) - u(x_0)| - |H(y_0 - x_0)| \Big|^p .$$

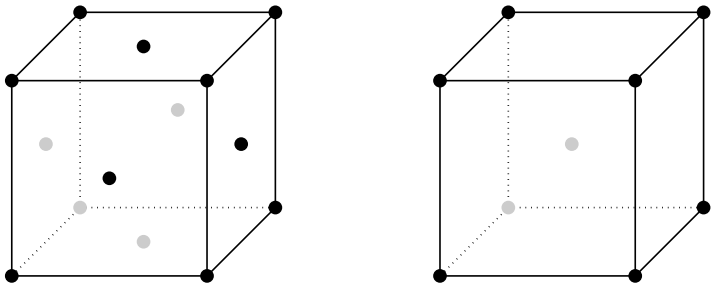
Lemma 2.3. *There exists a positive constant C_0 (depending on H) with the following property: if two neighbouring N-simplices S, T have different orientations in the deformed configuration, i.e.,*

$$\det(\nabla u|_S) \det(\nabla u|_T) \le 0 ,$$

then $E_{\text{cell}}(u; S \cup T) \ge C_0$.

Proof. We first consider the case when $H = I$ is the identity matrix. Let τ be a small positive constant. If $\max\{\operatorname{dist}(\nabla u|_S, O(N)), \operatorname{dist}(\nabla u|_T, O(N))\} > \tau$, then, by Lemma 2.2, $E_{\text{cell}}(u; S \cup T) \ge C\tau^p$. Otherwise we can assume that $\left|\nabla u|_T - I\right| < C\tau$ and $\left|\nabla u|_S - Q\right| < C\tau$, where $Q \in O(N) \backslash SO(N)$ is the reflection across the facet shared by S and T. If S and T are neighbouring simplices within the same unit cube, then $|x_0 - y_0| = \sqrt{2}$, since x_0 and y_0 are opposite vertices of a two-dimensional facet of the unit cube, while $|u(x_0) - u(y_0)| < C\tau$. This yields $E_{\text{cell}}(u; S \cup T) \ge 1$ for τ sufficiently small. If S and T belong to different cubes, then $|x_0 - y_0| = \sqrt{N - 1 + 4}$, while $|u(x_0) - u(y_0)| < \sqrt{N-1} + C\tau$, which gives $E_{\text{cell}}(u; S \cup T) \ge 1$ for small τ. The case of a general H is recovered by applying the previous argument to $v(x) := u(H^{-1}x)$. □

Remark 2.4. *For the sake of illustration, we show a detailed proof of Lemma 2.3 for $H = I$ in dimension two and three. In this remark, Q denotes a matrix as in the proof of Lemma 2.3.*



(a) (b)

Figure 3: Cubic cells of the face-centred cubic (a) and of the body-centred cubic lattice (b).

Let $N = 2$ and let $x_0, \dots, x_5$ be as in Figure 2(a). Let $T = [x_0, x_1, x_4]$ and $S = [x_0, x_4, x_5]$. In the case when $\left|\nabla u|_T - I\right| < C\tau$ and $\left|\nabla u|_S - Q\right| < C\tau$, we find that $|u(x_5) - u(x_1)| < C\tau$, which implies $E_{\text{cell}}(u; S \cup T) \geq 1$ for τ is sufficiently small. In the case when $T = [x_0, x_1, x_4]$, $S = [x_1, x_3, x_4]$, $\left|\nabla u|_T - I\right| < C\tau$, and $\left|\nabla u|_S - Q\right| < C\tau$, we have that $|u(x_3) - x_5| < C\tau$ (assuming w.l.o.g. that $u(x_4) = x_4$). Then $|u(x_3) - u(x_0)| < \sqrt{5} - 1$ and therefore $E_{\text{cell}}(u; S \cup T) \geq 1$ for small τ.

Let $N = 3$ and let $x_0, \dots, x_1 1$ be as in Figure 2(b). In the case when $T = [x_0, x_1, x_5, x_6]$, $S = [x_0, x_4, x_5, x_6]$, $\left|\nabla u|_T - I\right| < C\tau$, and $\left|\nabla u|_S - Q\right| < C\tau$, we have that $|u(x_4) - u(x_1)| < C\tau$, which yields $E_{\text{cell}}(u; S \cup T) \geq 1$. In the case when $T = [x_0, x_4, x_5, x_6]$, $S = [x_4, x_5, x_6, x_{10}]$, $\left|\nabla u|_T - I\right| < C\tau$, and $\left|\nabla u|_S - Q\right| < C\tau$, we have that $|u(x_{10}) - x_2| < C\tau$ (assuming w.l.o.g. that $u(x_6) = x_6$). Then $|u(x_0) - u(x_{10})| < \sqrt{6} - 1$, which gives $E_{\text{cell}}(u; S \cup T) \geq 1$ for τ small.

We conclude the discussion about discrete rigidity with some remarks on the choice of the interactions.

Remark 2.5. *For $N = 2$ and $H = I$, using the Kuhn decomposition we model a square lattice with bonds given by the sides and the diagonals of each cell. Notice that one of the diagonals is accounted for in B_1, while the other in B_2; the other bonds in B_2 correspond to longer range interactions. Further interactions could be added to the total energy in order to make the bonds symmetric. More precisely, one could define the total interaction energy as*

$$E(u; \Omega) := \sum_{\xi \in B(M)} \sum_{\substack{x \in \overline{\Omega} \cap \mathbb{Z}^N \\ x+\xi \in \overline{\Omega} \cap \mathbb{Z}^N}} \Big| |u(x+\xi) - u(x)| - |\xi| \Big|^p,$$

where $B(M) := \{\xi \in \mathbb{Z}^N : |\xi| \leq M\}$; for $M = \sqrt{3}$, $B(\sqrt{5}) \supset B_1 \cup B_2$. We underline that one retrieves the same rigidity properties stated above also by choosing $M = 2$; i.e., the Kuhn decomposition is not "optimal" in this case. In general, the choice of M depends on N and H.

The Kuhn decomposition is relevant especially for modeling some specific Bravais lattices as observed in the following remark.

Remark 2.6. *We show how the Kuhn decomposition can be used to parametrise Bravais lattices that are related with the crystalline structure of metals. We recall that a Bravais lattice in $\mathbb{R}^N$ consists of all integer combinations of N linearly independent vectors, called generators.*

For $N = 2$, the Bravais lattice generated by $v_1 = (1, 0)$ and $v_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$ is called (equilateral) triangular (or hexagonal) since every point has six nearest neighbours at distance one; moreover, every point has six next-to-nearest neighbours at distance $\sqrt{3}$. In order to map $\mathbb{Z}^2$ onto the triangular lattice, we set

$$H = \begin{pmatrix} 1 & -\frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix},$$

so that $He_1 = v_1$ and $H(e_1+e_2) = v_2$. One can see that H establishes a bijection between vectors in B_1, respectively B_2, and vectors associated with nearest neighbour interactions, respectively next-to-nearest, in the triangular lattice; cf. (1.1)–(1.2) *for the definition of B_1 and B_2.*

In dimension three, a structure of interest is the face-centred cubic lattice, which is the Bravais lattice generated by $v_1 = (0, \frac{1}{2}, \frac{1}{2})$, $v_2 = (\frac{1}{2}, 0, \frac{1}{2})$, and $v_3 = (\frac{1}{2}, \frac{1}{2}, 0)$; see Figure 3(a). Such lattice determines a subdivision of the space into cubic cells of edge one, where the atoms occupy the vertices and the centres of the facets of each cell. Each point has twelve nearest neighbours at distance $\frac{\sqrt{2}}{2}$ and six next-to-nearest neighbours at distance one. Nearest and next-to-nearest neighbour interactions guarantee the rigidity of the lattice; i.e., a deformation preserving the length of nearest and next-to-nearest bonds needs to be a rotation of the original lattice. Setting $He_1 = v_1$, $H(e_1 + e_2) = v_2$, and $H(e_1 + e_2 + e_3) = v_3$, we obtain

$$H = \tfrac{1}{2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 1 & 0 & -1 \end{pmatrix}.$$

Under this affinity, the bonds in B_1 associated with the Kuhn decomposition are transformed into twelve nearest and two next-to-nearest neighbour interactions for the face-centred cubic lattice; the images of the bonds in B_2 include four more next-to-nearest neighbour interactions. The total energy defined via the Kuhn decomposition includes few more interactions of longer range.

We conclude with the body-centred cubic lattice, which is generated by $v_1 = (-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$, $v_2 = (0, 0, 1)$, $v_3 = (0, 1, 0)$; see Figure 3(b). Here the atoms occupy the vertices and the centre of cubic cells of edge one. Arguing as above we get

$$H = \tfrac{1}{2} \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

Applying the transformation H, the fourteen bonds in B_1 are mapped into eight vectors of length $\frac{\sqrt{3}}{2}$ and six of length one; these correspond exactly to the nearest neighbour interactions in the body-centred cubic lattice, if the definition of the neighbours is based on a Delaunay triangulation, see [20] *for details. The twelve bonds in B_2 are in bijection with vectors corresponding to the next-to-nearest neighbour interactions for that triangulation.*

3. Compactness result

Before stating our main result, we recall that a partition $\{E_i\}_{i\in\mathbb{N}}$ of Ω is called a Caccioppoli partition if $\sum_{i\in\mathbb{N}} P(E_i, \Omega) < +\infty$, where $P(E_i, \Omega)$ denotes the perimeter of E_i in Ω. Given a rectifiable set $K \subset \Omega$, we say that a Caccioppoli partition $\{E_i\}_{i\in\mathbb{N}}$ of Ω is subordinated to K if for every $i \in \mathbb{N}$ the reduced boundary $\partial^* E_i$ of E_i is contained in K, up to a $\mathcal{H}^{N-1}$-negligible set.

Theorem 3.1 (Compactness)**.** *For every $\varepsilon > 0$ let $u_\varepsilon \in \mathcal{A}_\varepsilon$ be a sequence such that*

$$E_\varepsilon(u_\varepsilon) < C\,. \tag{3.1}$$

Then there exist a subsequence (not relabelled) and a function $u \in W^{1,\infty}(\Omega;\mathbb{R}^N)$ such that $\nabla u_\varepsilon \to \nabla u$ in $L^p(\Omega;\mathbb{M}^{N\times N})$ and

$$\nabla u \in SBV(\Omega;O(N)H)\,. \tag{3.2}$$

Specifically, u is a collection of an at most countable family of rigid deformations, i.e., there exists a Caccioppoli partition $\{E_i\}_{i\in\mathbb{N}}$ subordinated to the reduced boundary $\partial^*\{\nabla u \in SO(N)H\}$, such that

$$u(x) = \sum_{i\in\mathbb{N}} (R_i H x + b_i)\chi_{E_i}(x)\,, \tag{3.3}$$

where $R_i \in O(N)$ and $b_i \in \mathbb{R}^N$. Moreover, if $\partial^* E_i \cap \partial^* E_j \neq \emptyset$, then $\det R_i \det R_j = -1$ and $\partial^* E_i \cap \partial^* E_j$ is flat, i.e., the measure theoretic normal vector to $\partial^* E_i \cap \partial^* E_j$ is constant (up to the sign).

Proof. Note that by Lemma 2.2

$$\int_\Omega \operatorname{dist}^p(\nabla u_\varepsilon, O(N)H)\,\mathrm{d}x \le C\varepsilon\,. \tag{3.4}$$

In particular, $\|\nabla u_\varepsilon\|_{L^p(\Omega)} < C$ and therefore, up to subsequences, $u_\varepsilon - \fint_\Omega u_\varepsilon\,\mathrm{d}x \rightharpoonup u$ weakly in $W^{1,p}(\Omega;\mathbb{R}^N)$, for some $u \in W^{1,p}(\Omega;\mathbb{R}^N)$. We first prove that $\nabla u \in O(N)H$ (which implies that $u \in W^{1,\infty}(\Omega;\mathbb{R}^N)$) and then that $\nabla u_\varepsilon \to \nabla u$ strongly in $L^p(\Omega)$.

Introduce the function $s_\varepsilon : \Omega \to \{-1,1\}$ defined by

$$s_\varepsilon(x) := \begin{cases} 1 & \text{in } \Omega_\varepsilon^+\,,\\ -1 & \text{in } \Omega_\varepsilon^-\,,\end{cases}$$

where $\Omega_\varepsilon^+ := \{\det \nabla u_\varepsilon \ge 0\}$ and $\Omega_\varepsilon^- := \{\det \nabla u_\varepsilon < 0\}$. Remark that $s_\varepsilon \in BV(\Omega;\{\pm 1\})$ and, by (3.1) and Lemma 2.3, J_{s_ε} is the union of C/ε^{N-1} facets of $(N-1)$-dimensional measure of order ε^{N-1}, whence

$$\mathcal{H}^{N-1}(J_{s_\varepsilon}) < C \quad \text{uniformly in } \varepsilon\,.$$

Therefore, applying standard compactness results for sets of finite perimeter (see [3]), we can extract a subsequence s_ε (not relabelled) converging to a function $s \in BV(\Omega;\{\pm 1\})$ strongly in $L^1(\Omega)$. Let $\bar x \in \Omega$ be a Lebesgue point for both ∇u and s and let $B_r(\bar x)$ denote the ball of radius r and centre $\bar x$. Assume that the Lebesgue value of s at $\bar x$ is 1. Then, by Theorem 2.1, (3.4), and the fact that the maximum distance between matrices in $O(N)$ and $SO(N)$ is bounded, one finds

$$\begin{aligned} &\fint_{B_r(\bar x)} |\nabla u_\varepsilon - R_\varepsilon^r H|^p\,\mathrm{d}x \le C \fint_{B_r(\bar x)} \operatorname{dist}^p(\nabla u_\varepsilon, SO(N)H)\,\mathrm{d}x\\ &\le C \fint_{B_r(\bar x)} \big(\operatorname{dist}^p(\nabla u_\varepsilon, O(N)H) + |s_\varepsilon(x)-1|\big)\,\mathrm{d}x \le Cr^{-N}\varepsilon + C\fint_{B_r(\bar x)} |s_\varepsilon(x)-1|\,\mathrm{d}x\,, \end{aligned} \tag{3.5}$$

for some $R_\varepsilon^r \in SO(N)$. Using the strong convergence of s_ε to s in L^1, up to extracting a further subsequence, one can pass to the limit as $\varepsilon \to 0$ in (3.5) and get

$$\fint_{B_r(\bar x)} |\nabla u - R^r H|^p\,\mathrm{d}x \le C \fint_{B_r(\bar x)} |s(x)-1|\,\mathrm{d}x\,, \tag{3.6}$$

where $R^r \in SO(N)$. Letting $r \to 0$ in (3.6), and possibly extracting a further subsequence, we deduce that the Lebesgue value of ∇u at $\bar x$ is RH for some $R \in SO(N)$. Therefore the Lebesgue

value of ∇u at every Lebesgue point where $\tilde{s} = 1$ (where $\tilde{s}$ is the Lebesgue representative of s) is an element of $SO(N)H$. We apply the same argument to Qu_ε, where $Q \in O(N)\backslash SO(N)$ is any fixed rotoreflection, to find that the Lebesgue value of ∇u at every Lebesgue point where $\tilde{s} = -1$ is an element of $(O(N)\backslash SO(N))H$. Moreover the set $\{\nabla u \in SO(N)H\}$ is of finite perimeter in Ω, since $s \in BV(\Omega; \{\pm 1\})$.

In order to show the strong convergence, we will show that the L^p norm is conserved, namely,

$$\lim_{\varepsilon\to 0^+} \int_\Omega |\nabla u_\varepsilon|^p \,\mathrm{d}x = \int_\Omega |\nabla u|^p \,\mathrm{d}x\,.$$

Fix $\eta > 0$ and let $\Omega_\varepsilon^\eta := \big\{\mathrm{dist}(\nabla u_\varepsilon, O(N)H) > \eta\big\}$. Since $|\Omega_\varepsilon^\eta| \to 0$ in measure, one has that

$$\int_{\Omega_\varepsilon^\eta} |\nabla u_\varepsilon|^p \,\mathrm{d}x \le C \int_{\Omega_\varepsilon^\eta} \mathrm{dist}^p(\nabla u_\varepsilon, O(N)H)\,\mathrm{d}x + C|\Omega_\varepsilon^\eta| \le C\big(\varepsilon E_\varepsilon + |\Omega_\varepsilon^\eta|\big) \to 0\,.$$

Then

$$\begin{aligned}\int_\Omega |\nabla u_\varepsilon|^p \,\mathrm{d}x &= \int_{\Omega_\varepsilon^\eta} |\nabla u_\varepsilon|^p \,\mathrm{d}x + \int_{\Omega\setminus\Omega_\varepsilon^\eta} |\nabla u_\varepsilon|^p \,\mathrm{d}x = o(1) + (N^{p/2} + \sigma(\eta))|\Omega \setminus \Omega_\varepsilon^\eta| \\ &\to (N^{p/2} + \sigma(\eta)) = \int_\Omega |\nabla u|^p \,\mathrm{d}x + \sigma(\eta)\,,\end{aligned}$$

with $\sigma(\eta) \to 0$ as $\eta \to 0^+$.

Finally, we prove that u is a collection of an at most countable family of rigid deformations. To this end, fix $Q \in O(N) \setminus SO(N)$ and define

$$v := \begin{cases} u & \text{if } \nabla u \in SO(N)H\,, \\ Qu & \text{if } \nabla u \in (O(N)\backslash SO(N))H\,. \end{cases}$$

Since $v \in SBV(\Omega;\mathbb{R}^N)$ and $\nabla v \in SO(N)H$ a.e. in Ω, we can appeal to [12, Theorem 1.1] and deduce that there exists a Caccioppoli partition $\{E_i\}_{i\in\mathbb{N}}$ subordinated to J_v, such that

$$v(x) = \sum_{i\in\mathbb{N}} (R_i H x + b_i)\chi_{E_i}(x)\,,$$

where $R_i \in SO(N)$ and $b_i \in \mathbb{R}^N$. Taking into account that $\{\nabla u \in SO(N)H\}$ has finite perimeter, this implies (3.2) and (3.3). The last part of the statement follows from Lemma 3.2 below. □

Lemma 3.2. *Let $\Omega \subset \mathbb{R}^N$ be an open, bounded set with Lipschitz boundary, and let $u \in W^{1,\infty}(\Omega;\mathbb{R}^N)$. Suppose that there exists a Caccioppoli partition $\{E_i\}_{i\in\mathbb{N}}$ of Ω such that*

$$u(x) = \sum_{i\in\mathbb{N}} (P_i x + b_i)\chi_{E_i}(x)\,,$$

where $P_i \in \mathbb{M}^{N\times N}$ and $b_i \in \mathbb{R}^N$. If $\partial^* E_i \cap \partial^* E_j \neq \emptyset$, then $\mathrm{rank}(P_i - P_j) \le 1$ and, denoted by ν_i the measure theoretic inner normal to E_i, ν_i is constant on $\partial^* E_i \cap \partial^* E_j$.

Proof. Let $\bar{x} \in \partial^* E_i \cap \partial^* E_j$. Then $\bar{x} \in J_{\nabla u}$, i.e., there exists a unit vector $\nu \in \mathbb{R}^N$ such that

$$\lim_{\varepsilon\to 0^+} \fint_{B_\varepsilon^{\nu+}(\bar{x})} |\nabla v - P_i|\,\mathrm{d}x = 0\,, \quad \lim_{\varepsilon\to 0^+} \fint_{B_\varepsilon^{\nu-}(\bar{x})} |\nabla v - P_j|\,\mathrm{d}x = 0\,, \tag{3.7}$$

where $B_\varepsilon^{\nu\pm}(\bar{x}) := B_\varepsilon(\bar{x}) \cap \{x\colon \pm\, x\cdot\nu > 0\}$ and $B_r(p)$ denotes the ball of radius r and centre p; cf. [3, Definition 3.67 and Example 3.68]. For $x \in B_1(0)$ define the sequence $v_\varepsilon(x) := \frac{1}{\varepsilon} v(\varepsilon(x - \bar{x}))$. Then $\nabla v_\varepsilon(x) = \nabla v(\varepsilon(x-\bar{x}))$ and, by (3.7), we have that $\nabla v_\varepsilon \to \chi P_i + (1-\chi)P_j$

in $L^p(B_1(0);\mathbb{M}^{N\times N})$ for every $p\geq 1$, where χ is the characteristic function of $B_1^{\nu+}(0)$. The thesis now follows from the rigidity of the two-gradient problem, see e.g. [21, Proposition 2.1]. □

4. Lower and upper bounds

In this section we provide lower and upper bounds for the Γ-limit of (any subsequence of) $\{E_\varepsilon\}$ in terms of interfacial energies that penalise changes of orientation. In what follows we denote by $E'(\cdot)$ and $E''(\cdot)$ the Γ-lim inf and the Γ-lim sup as $\varepsilon\to 0^+$, respectively, of the sequence $\{E_\varepsilon\}$ with respect to the strong convergence in $W^{1,p}(\Omega;\mathbb{R}^N)$. We also introduce a "localised" version of the functionals E_ε by setting, for any open set $A\subset\mathbb{R}^N$,

$$E_\varepsilon(u;A)=\varepsilon^{N-1}\sum_{\xi\in B_1\cup B_2}\sum_{\substack{x\in\varepsilon\mathbb{Z}^N\cap A\\ x+\varepsilon\xi\in\varepsilon\mathbb{Z}^N\cap A}}\left|\frac{|u(x+\varepsilon\xi)-u(x)|}{\varepsilon}-|H\xi|\right|^p.$$

Moreover, given ν in the unit sphere S^{N-1}, we denote by Q_ν any cube centred at 0, with side length 1 and two faces orthogonal to ν, and by u_0^ν the piecewise affine function defined by

$$u_0^\nu(x):=\begin{cases}Hx & \text{if } \langle x,\nu\rangle\geq 0\,,\\ R_\nu x & \text{otherwise,}\end{cases}$$

where $R_\nu\in(O(N)\backslash SO(N))H$ is such that $H-R_\nu=a\otimes\nu$ for some $a\in\mathbb{R}^N$.

Proposition 4.1 (Lower bound)**.** *For every $u\in W^{1,\infty}(\Omega;\mathbb{R}^N)$ with $\nabla u\in SBV(\Omega;O(N)H)$, one has*

$$E'(u)\geq\int_{J_{\nabla u}}g_1(\nu_{\nabla u})\,\mathrm{d}\mathcal{H}^{N-1}\,,$$

where $g_1:S^{N-1}\to[0,+\infty)$ is defined by

$$g_1(\nu):=\inf\Big\{\liminf_{n\to\infty}E_{\varepsilon_n}(u_n;Q_\nu)\colon \varepsilon_n\to 0\,,\ u_n\to u_0^\nu \text{ strongly in } W^{1,p}(Q_\nu;\mathbb{R}^N)\Big\}\,,$$

and satisfies $g_1(\nu)=g_1(-\nu)$.

Proof. Suppose that $u_\varepsilon\to u$ in $W^{1,p}(Q_\nu;\mathbb{R}^N)$ and $\sup_\varepsilon E_\varepsilon(u_\varepsilon)<+\infty$. Let

$$r:=\sup\{|\xi|\colon \xi\in B_1\cup B_2\}\,, \tag{4.1}$$

and define the family of positive measures

$$\mu_\varepsilon:=\sum_{x\in\mathcal{L}_\varepsilon^r}\left(\sum_{\xi\in B_1\cup B_2}\left|\frac{|u_\varepsilon(x+\varepsilon\xi)-u_\varepsilon(x)|}{\varepsilon}-|H\xi|\right|^p\right)\delta_x\,,$$

where $\mathcal{L}_\varepsilon^r=\{x\in\mathcal{L}_\varepsilon\colon \operatorname{dist}(x,\partial\Omega)\geq r\varepsilon\}$. Note that

$$E_\varepsilon(u_\varepsilon)\geq\mu_\varepsilon(\Omega)\,,$$

hence, up to passing to a subsequence, we may suppose that there exists a positive measure μ such that $\mu_\varepsilon\overset{*}{\rightharpoonup}\mu$. We now use a blow-up argument. By the Radon-Nikodym Theorem, we can decompose μ into two mutually singular positive measures:

$$\mu=g\,\mathcal{H}^{N-1}\llcorner J_{\nabla u}+\mu^s\,.$$

We complete the proof if we show that

$$g(x_0)\geq g_1(\nu_{\nabla u}(x_0))\quad\text{for } \mathcal{H}^{N-1}\text{-a.e. } x_0\in J_{\nabla u}\,.$$

By the properties of BV functions we know that for $\mathcal{H}^{N-1}$-a.e. $x_0 \in J_{\nabla u}$

(i) $\lim_{\rho\to 0} \frac{1}{\rho^{N-1}} \mathcal{H}^{N-1}(J_{\nabla u} \cap (x_0 + \rho Q_{\nu_{\nabla u}(x_0)})) = 1\,,$

(ii) $\lim_{\rho\to 0} \frac{1}{\rho^N} \int_{\rho Q^{\pm}_{\nu_{\nabla u}(x_0)}} |\nabla u(y) - \nabla u^{\pm}(x_0)|\,\mathrm{d}x = 0\,,$

(iii) $g(x_0) = \lim_{\rho\to 0} \frac{\mu(x_0 + \rho Q_{\nu_{\nabla u}(x_0)})}{\mathcal{H}^{N-1}(J_{\nabla u} \cap (x_0 + \rho Q_{\nu_{\nabla u}(x_0)}))}\,.$

Fix such a point $x_0 \in J_{\nabla u}$ and let $\{\rho_n\}$ be a sequence of positive numbers converging to zero such that $\mu(x_0 + \rho_n \partial Q_{\nu_{\nabla u}(x_0)}) = 0$. From (i) and (iii) it follows that

$$g(x_0) = \lim_{n\to\infty} \lim_{\varepsilon\to 0} \frac{1}{\rho_n^{N-1}} \mu_\varepsilon(x_0 + \rho_n Q_{\nu_{\nabla u}(x_0)})\,.$$

Note that for every $\varepsilon > 0$ and $n \in \mathbb{N}$ we can find $\rho_{n,\varepsilon}$ and $x_{0,\varepsilon} \in \varepsilon\mathbb{Z}^N$ such that $\lim_{\varepsilon\to 0} \rho_{n,\varepsilon} = \rho_n$, $\lim_{\varepsilon\to 0} x_{0,\varepsilon} = x_0$, and

$$x_0 + (\rho_n - R\varepsilon)\, Q_{\nu_{\nabla u}(x_0)} \supseteq x_{0,\varepsilon} + \rho_{n,\varepsilon} Q_{\nu_{\nabla u}(x_0)}\,.$$

Then

$$g(x_0) \geq \lim_{n\to\infty} \lim_{\varepsilon\to 0} \frac{1}{\rho_{n,\varepsilon}^{N-1}} E_\varepsilon(u_\varepsilon; x_{0,\varepsilon} + \rho_{n,\varepsilon} Q_{\nu_{\nabla u}(x_0)})\,.$$

Set

$$u_{n,\varepsilon}(x) := u_\varepsilon(x_{0,\varepsilon} + \rho_{n,\varepsilon} x) \quad \text{for } x \in \frac{\varepsilon}{\rho_{n,\varepsilon}}\mathbb{Z}^N\,,$$
$$v_{n,\varepsilon} := u_{n,\varepsilon} - c_{n,\varepsilon}\,,$$
$$F^{\pm} := \nabla u^{\pm}(x_0)\,.$$

Since $u_\varepsilon \to u$ in $W^{1,p}(\Omega;\mathbb{R}^N)$, from (ii) we deduce that there exist constants $c_{n,\varepsilon}$ such that

$$\lim_{n\to\infty} \lim_{\varepsilon\to 0} \|v_{n,\varepsilon} - u_{F^+,F^-}\|_{W^{1,p}(Q_{\nu_{\nabla u}(x_0)};\mathbb{R}^N)} = 0\,,$$

where

$$u_{F^+,F^-}(x) := \begin{cases} F^+ x & \text{if } \langle x, \nu\rangle \geq 0\,, \\ F^- x & \text{otherwise.} \end{cases}$$

Using a standard diagonalisation argument and the translational invariance of E_ε with respect to both independent and dependent variables, we can find a sequence of positive numbers $\lambda_k \to 0$ and a sequence v_k converging to u_{F^+,F^-} in $W^{1,p}(Q_{\nu_{\nabla u}(x_0)};\mathbb{R}^N)$ such that

$$g(x_0) \geq \lim_{k\to\infty} E_{\lambda_k}(v_k; Q_{\nu_{\nabla u}(x_0)})\,.$$

The conclusion then follows by the very definition of g_1 and taking into account that, by invariance with respect to $O(N)$, we may replace v_k by Rv_k, $R \in O(N)$, without changing the energy. □

Remark 4.2. *By a slicing argument, we may show that*

$$\inf_{\nu\in S^{N-1}} g_1(\nu) \geq \frac{C_0}{N} > 0\,, \tag{4.2}$$

where C_0 is as in Lemma 2.3. This implies in particular that

$$E'(u) \geq \frac{C_0}{N}\, \mathcal{H}^{N-1}(J_{\nabla u})\,.$$

In order to prove (4.2)*, let us set, for every* $k \in \{1, \dots, N\}$*,*

$$S^k_\nu := \Pi^{e_k}(Q_\nu \cap \{\langle x, \nu\rangle = 0\})\,,$$

where Π^{e_k} *denote the orthogonal projection on* $\{\langle x, e_k\rangle = 0\}$*. Let* $\varepsilon_n \to 0$ *and* $u_n \to u^\nu_0$ *strongly in* $W^{1,p}(Q_\nu;\mathbb{R}^N)$*, and for any* $k \in \{1, \dots, N\}$ *set*

$$I^k_n := I^{k+}_n \cup I^{k-}_n\,,$$

where

$$I^{k\pm}_n := \{i \in \varepsilon\mathbb{Z}^N \cap S^k_\nu \colon \pm \det \nabla u_n(x) > 0 \ \forall\, x \in ((\Pi^{e_k})^{-1}(i) + [0,\varepsilon_n]^N) \cap Q_\nu\}\,.$$

Then, one easily gets that

$$\int_{Q_\nu} |\nabla u_n - \nabla u^\nu_0|^p \,\mathrm{d}x \geq C\varepsilon^{N-1}\#I^k_n + o(1)\,,$$

so that $\varepsilon^{N-1}\#I^k_n \to 0$*. Hence, by Lemma 2.3 we deduce that*

$$\liminf_{n\to\infty} E_{\varepsilon_n}(u_n, Q_\nu) \geq C_0 \max_{k=1,\dots,N} \liminf_{n\to\infty} \varepsilon_n^{N-1}\#(I^k_n)^c = C_0 \max_{k=1,\dots,N} |S^k_\nu| \geq \frac{C_0}{N}\,.$$

Remark 4.3. *A slicing argument can be also exploited to obtain a more refined lower bound on* g_1 *in terms of minimum problems for one-dimensional energies. For example, if* $N = 2$ *and* H *is as in Remark 2.6 (and thus we are modeling a triangular lattice with nearest and next-to-nearest neighbour interactions), we can bound* g_1 *from below by means of minimum problems for p-harmonic nearest and next-to-nearest neighbour interactions in one dimension, which can be analysed following the approach developed in* [13] *and* [6]*. Precisely, if* $N = 2$ *and* H *is as in Remark 2.6, we get that the sets* B_1 *and* B_2 *defined in* (1.1) *and* (1.2) *are given by*

$$B_1 = \{\pm v_1, \pm v_2, \pm v_3\}\,,$$

where $v_1 := (1,0)$*,* $v_2 := (0,1)$*,* $v_3 := (1,1)$*, and*

$$B_2 = \{\pm \xi_1, \pm \xi_2, \pm \xi_3\}\,,$$

where $\xi_1 := (1,2)$*,* $\xi_2 := (2,1)$*,* $\xi_3 := (-1,1)$*. Note that, by regrouping the energetic contributions of the interactions and neglecting the interactions near the boundary, we get that for any* $Q' \subset\subset Q_\nu$

$$E_\varepsilon(u; Q_\nu) \geq \sum_{i=1}^3 E^i_\varepsilon(u; Q')\,,$$

where

$$E^i_\varepsilon(u; Q') = \varepsilon \sum_{\xi\in C_i} c(\xi) \sum_{\substack{x\in\varepsilon\mathbb{Z}^2\cap Q'\\ x+\varepsilon\xi\in\varepsilon\mathbb{Z}^2\cap Q'}} \Big|\frac{|u(x+\varepsilon\xi)-u(x)|}{\varepsilon} - |H\xi|\Big|^p\,,$$

with

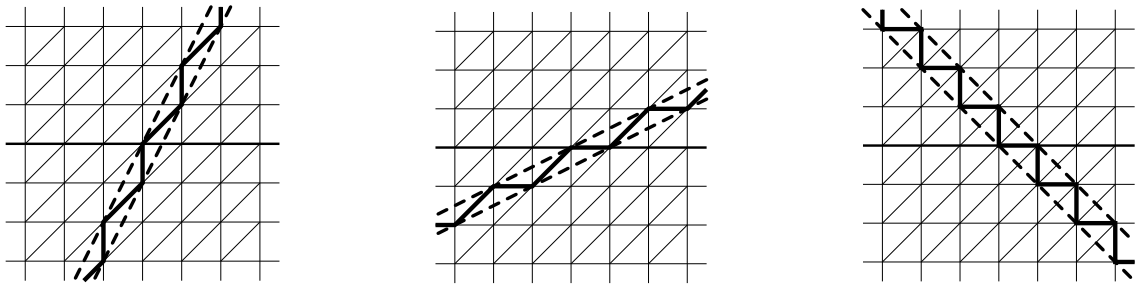
$$C_1 := \{\pm\xi_1, \pm v_2, \pm v_3\}\,, \quad C_2 := \{\pm\xi_2, \pm v_1, \pm v_3\}\,, \quad C_3 := \{\pm\xi_3, \pm v_1, \pm v_2\}\,,$$

and

$$c(\xi) := \begin{cases} 1 & \text{if } \xi \in B_2\,,\\ 1/2 & \text{if } \xi \in B_1\,. \end{cases}$$

Let us introduce the infinite chains of particles defined by

$$\mathcal{Z}_1 := \mathbb{Z}\xi_1 \cup (\mathbb{Z}\xi_1 + v_3)\,, \quad \mathcal{Z}_2 := \mathbb{Z}\xi_2 \cup (\mathbb{Z}\xi_2 + v_1)\,, \quad \mathcal{Z}_3 := \mathbb{Z}\xi_3 \cup (\mathbb{Z}\xi_3 + v_2)$$



(a) (b) (c)

Figure 4: The bold zig-zag lines describe the chains of particles $\mathcal{Z}_i$, $i = 1, 2, 3$ (cf. Remark 4.3). The dashed lines are aligned with the vectors ξ_i and interpolate next-to-nearest neighbours. The horizontal bold line represents the interface corresponding to $\nu = e_2$.

(see Figure 4). Given $L \in \mathbb{N}$, set

$$\mathcal{Z}_i^L = \mathcal{Z}_i \cap \{x \in \mathbb{R}^2 \colon |x \cdot \xi_i| \leq L|\xi_i|\}, \quad i = 1, 2, 3\,.$$

We can then introduce, for any $i \in \{1, 2, 3\}$ and $L \in \mathbb{N}$, a one-dimensional energy accounting for nearest and next-to-nearest neighbour interactions defined on the maps $u \colon \mathcal{Z}_i^L \to \mathbb{R}^2$ as

$$E^{i,L}(u) := \frac{1}{2} \sum_{\xi \in C_i} \sum_{\substack{x \in \mathcal{Z}_i^L \\ x+\xi \in \mathcal{Z}_i^L}} \Big| |u(x+\xi) - u(x)| - |H\xi| \Big|^p .$$

Using a slicing procedure, we may then deduce that

$$g_1(\nu) \geq \sum_{i=1}^{3} m_i(\nu) |\nu \cdot \xi_i|\,,$$

where

$$m_i(\nu) = \inf_{L \in \mathbb{N}} \inf \left\{ E^{i,L}(u) \colon u(x) = u_0^\nu(x) \text{ if } (L-1)|\xi_i| \leq |x \cdot \xi_i| \leq L|\xi_i| \right\}.$$

We now provide an upper estimate of $E''(u)$ for a suitable subclass of the limiting deformations u identified by Theorem 3.1. We say that a set $K \subset \Omega$ is polyhedral with respect to Ω if it consists of the intersection of Ω with the union of a finite number of $(N-1)$-dimensional simplices of $\mathbb{R}^N$. We set then

$$\mathcal{W}(\Omega) := \{u \in W^{1,\infty}(\Omega; \mathbb{R}^N) \colon \nabla u \in SBV(\Omega; O(N)H) \text{ and } J_{\nabla u} \text{ is polyhedral in } \Omega\}\,.$$

Proposition 4.4 (Upper bound)**.** *For any $u \in \mathcal{W}(\Omega)$, the following inequality holds true:*

$$E''(u) \leq \int_{J_{\nabla u}} g_2(\nu_{\nabla u})\, \mathrm{d}\mathcal{H}^{N-1}\,,$$

where, $g_2 : S^{N-1} \to [0, +\infty)$ is defined by

$$g_2(\nu) := \lim_{T \to \infty} \frac{1}{T^{N-1}} \inf\{E_1(u; TQ_\nu) \colon u(x) = u_0^\nu(x) \text{ if } \operatorname{dist}(x, \partial(TQ_\nu)) \leq r\}\,, \tag{4.3}$$

and r is given by (4.1)*.*

Proof. We analyse only the case where $J_{\nabla u}$ is the restriction to Ω of a hyperplane, since the case of a general polyhedral boundary is easily recovered by a gluing argument. Fix then $\nu \in S^{N-1}$, let $J_{\nabla u} = \Pi_\nu \cap \Omega$, where Π_ν is a hyperplane orthogonal to ν. By translational and rotational invariance, without loss of generality we may assume that $\Pi_\nu = \{x \in \mathbb{R}^N \colon \langle x, \nu\rangle = 0\}$ and $u = u_0^\nu$. Given $\delta > 0$, let $T_\delta > 0$ and u_δ such that $u_\delta(x) = u_0^\nu(x)$ if $\operatorname{dist}(x, \partial(T_\delta Q_\nu)) \le r$ and

$$\frac{1}{T_\delta^{N-1}} E_1(u_\delta; T_\delta Q_\nu) \le g_2(\nu) + \delta\,.$$

Let $\{b_1, \dots, b_N\}$ be an orthonormal base of $\mathbb{R}^N$ such that $b_N = \nu$ and $Q_\nu = \{x \in \mathbb{R}^N \colon |\langle x, b_l\rangle| < 1/2\,,\ l = 1, \dots, N\}$. For any $j \in \bigoplus_{l=1}^{N-1} \mathbb{Z} T_\delta b_l$ set $x_j = [j] = ([j_1], \dots, [j_N])$, where $[\cdot]$ denotes the integer part. Then let $u_\varepsilon \colon \varepsilon\mathbb{Z}^N \cap \Omega \to \mathbb{R}^N$ be such that

$$u_\varepsilon(\varepsilon i) = u_\delta(i - x_j) + \varepsilon H x_j \quad \text{for } i \in \mathbb{Z}^N \cap T_\delta Q_\nu + x_j\,,\ j \in \bigoplus_{l=1}^{N-1} \mathbb{Z}(T_\delta + 2r) b_l\,,$$

and $u \equiv u_0^\nu$ otherwise. Then $u_\varepsilon \to u$ strongly in $W^{1,p}(\Omega; \mathbb{R}^N)$ and

$$E''(u) \le \limsup_{\varepsilon \to 0} E_\varepsilon(u_\varepsilon) \le \frac{\mathcal{H}^{N-1}(J_{\nabla u})}{T_\delta^{N-1}} E_1(u_\delta; T_\delta Q_\nu) + O(\delta) \le (g_2(\nu) + \delta)\mathcal{H}^{N-1}(J_{\nabla u}) + O(\delta)\,.$$

The conclusion follows by letting δ tend to 0. □

Remark 4.5. *Testing the infimum problems defining g_2 with $u = u_0^\nu$, we easily get that $g_2(\nu) \le C$ uniformly in ν. In particular, we have that for every $u \in \mathcal{W}(\Omega)$*

$$E''(u) \le C\mathcal{H}^{N-1}(J_{\nabla u})\,.$$

Explicit estimates on g_2 can be given for example in the particular case of a two-dimensional triangular lattice, see Remark 2.6, when ν is orthogonal to a lattice direction, specifically $\nu \in \{(0,1), (-\frac{\sqrt{3}}{2}, \frac{1}{2}), (\frac{\sqrt{3}}{2}, \frac{1}{2})\}$. One can easily see that $g_2((0,1)) = g_2((-\frac{\sqrt{3}}{2}, \frac{1}{2})) = g_2((\frac{\sqrt{3}}{2}, \frac{1}{2})) \le 3^{\frac{p}{2}}$. Indeed, the only active bonds are the next-to-nearest neighbour bonds across the interface, whose cardinality is of order T, cfr. (4.3).

Remark 4.6. *The computation of the Γ-limit of E_ε remains an open question. However, we believe that the bounds provided in Propositions 4.1 and 4.4 give some insight into its derivation. Assume that the following result holds true: given any test sequence u_n in the definition of g_1, there exists a sequence of functions v_n such that $v_n \to u_0^\nu$ strongly in $W^{1,p}(Q_\nu, \mathbb{R}^N)$, $v_n(x) = u_0^\nu(x)$ if $\operatorname{dist}(x, \partial(T_\delta Q_\nu)) \le r$ and $E_{\varepsilon_n}(v_n; Q_\nu) \le E_{\varepsilon_n}(u_n; Q_\nu) + o(1)$. Then it could be easily shown that $g_1 = g_2$ and, consequently, the interfacial energies in Propositions 4.1 and 4.4 would provide the Γ-limit of $E_\varepsilon(u)$ for any $u \in \mathcal{W}(\Omega)$.*

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